

Magnetization and Lyapunov exponents on a kagome chain with multi-site exchange interaction

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Abstract

The Ising approximation of the Heisenberg model in a strong magnetic field, with two, three and six spin exchange interactions is studied on a kagome chain. The kagome chain can be considered as an approximation of the third layer of ^3He absorbed on the surface of graphite (kagome lattice). By using dynamical approach we have found one and multi-dimensional mappings (recursion relations) for the partition function. The magnetization diagrams are plotted and they show that the kagome chain is separating into four sublattices with different magnetizations. Magnetization curves of two sublattices exhibit plateaus at zero and $2/3$ of the saturation field. The maximal Lyapunov exponent for multi-dimensional mapping is considered and it is shown that near the magnetization plateaus the maximal Lyapunov exponent also exhibits plateaus.

Key words: Multiple spin exchange, solid and fluid ^3He , recursive lattice, dynamical systems, magnetization plateau, antiferromagnetic Ising model, kagome chain

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1. Introduction

The partition function of a statistical system can be calculated by means of several methods: transfer matrix approach [1], dynamic technique [2]-[4] etc. The most useful for recursive lattices is the dynamical approach, which is a very powerful tool for research of a number of theoretical problems in statistical mechanics. By means of this approach one can obtain exact recursive relations for the partition function on recurrent lattices.

As the systems of almost localized identical fermions one can model solid and fluid ^3He films. Since the light mass spin- $1/2$ ^3He atoms are subject to a weak attractive potential, the theoretical explanation of magnetism is based on the multiple-spin exchange mechanism [5]. An important case is represented by solid and fluid ^3He films absorbed on the surface of graphite [6, 7, 8] since it is a typical example of a two-dimensional frustrated quantum-spin system [9]. The first and second layers of the system form a triangular lattice, while the third one forms a system of quantum $1/2$ spins on a kagome lattice [10].

In a strong external magnetic field Heisenberg model can be approximated by the Ising one. If the strong magnetic field is directed along the z -axis, a reduction of transverse fluctuations is expected to occur; it is supposed that in this case σ^x and σ^y -spin components are infinitely small and may be neglected [5, 11].

The phenomenon of magnetization plateau has been studied during the past decade both experimentally and theoretically. The plateaus may be exhibited in the magnetization curves of quantum spin systems at very low temperatures in case of strong external fields. The plateaus of this kind were first observed by Hida [12] in trimerized $S=1/2$ spin chains and they were analytically explained by Okamoto [13]. Magnetization plateaus appear in a wide range of models on chains, ladders, hierarchical lattices, theoretically analysed

by dynamical, transfer matrix approaches and exact diagonalization in clusters (see Ref. [14]-[26]). The experimental evidence for the appearance of magnetization plateaus has also been found for two-dimensional systems [27]-[30]. On triangular lattices a magnetization plateau was observed at $m/m_s = 1/3$ for compounds like C_6Eu [31], $CsCuCl_3$ [32] (see also Ref. [33]-[35]); plateaus have also been observed on a kagome lattice (see Ref. [36]-[40]).

In the present paper the dynamical (recursive) approach was used to study magnetic properties of a kagome chain. The magnetization plateaus were found at low temperatures and moreover, the kagome chain was separated into four sublattices with different magnetizations. Two of these exhibited plateaus, whereas the others did not. The stability of the system is described by Lyapunov exponents [41] by means of which the exponential rate is measured, at which the adjacent orbits converge or diverge [42]-[44]. It is interesting to check whether the maximum Lyapunov exponent has plateaus that coincide with the magnetization one.

This paper is organized as follows: in Section 2 the two, three and six-site exchange interactions in a strong magnetic field are described, in Section 3 the exact recursion relation for the partition function is derived, the magnetization curves for different values of temperature and exchange parameters are displayed in Section 4. In Section 5 a multidimensional mapping for the partition function is obtained and the corresponding maximum Lyapunov exponent is investigated. Finally, Section 6 contains the concluding remarks.

2. Exchange Hamiltonian with two, three and six- site exchange

The Heisenberg Hamiltonian for kagome chain consists of two parts

$$H = H_{ex} + H_Z, \quad (1)$$

where H_{ex} is the spin exchange Hamiltonian and H_Z is the Zeeman Hamiltonian which is responsible for magnetism, which has the following form

$$H_Z = - \sum_i \frac{\gamma}{2} \hbar \mathbf{B} \boldsymbol{\sigma}_i = -h \sum_i \sigma_i, \quad (2)$$

where γ is the gyromagnetic ratio for a nucleus, and \mathbf{B} is the magnetic field [5].

According to [5] the multiple spin exchanges Hamiltonian can be written as

$$H_{ex} = J_2 \sum_{Pairs} P_2 - J_3 \sum_{Triangles} (P_3 + P_3^{-1}) + J_6 \sum_{Hexagons} (P_6 + P_6^{-1}), \quad (3)$$

where P_2 is the pair transposition operator, P_3 (P_6) is the operator making a cyclic rearrangement in the triangle (hexagon). The explicit expression of pair transposition operator P_{ij} was been given by Dirac

$$P_2 \equiv P_{ij} = \frac{1}{2} (1 + \boldsymbol{\sigma}_i \boldsymbol{\sigma}_j), \quad (4)$$

where $\boldsymbol{\sigma}_i$ is the Pauli matrix, acting on the spin at the i -th site. The expressions for P_3 , and P_6 in terms of Pauli matrixes were derived in [23]. By using these expressions one can rewrite the Heisenberg Hamiltonian in terms of Pauli matrices. By taking into account that in a strong external magnetic field directed along the z -axis the contribution from x and y spin component will be negligible and the only relevant contribution will come from the z component (which can effectively take values $s_z = \pm 1$), we may consider an Ising model instead of Heisenberg one. By using expressions for P_3 , and P_6 and by substituting the Pauli matrix with s_z we get the Ising approximation of the Heisenberg Hamiltonian:

$$H = \frac{J_2}{2} \sum_{Pairs} (1 + s_i s_j) - \frac{J_3}{2} \sum_{Triangles} (1 + s_i s_j + s_j s_k + s_k s_i) + \frac{J_6}{2} \sum_{Hexagons} H^{(6)} - h \sum_i s_i, \quad (5)$$

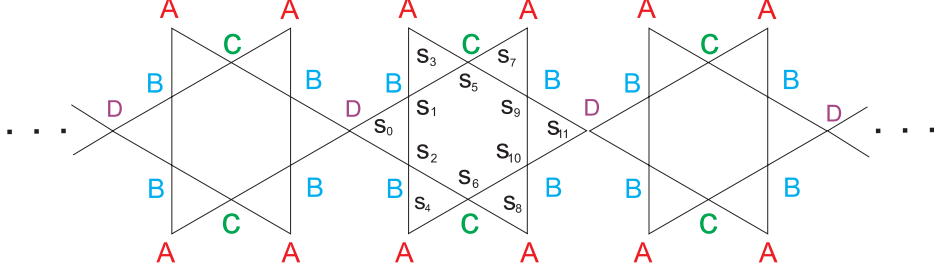


Figure 1: Sublattices on the kagome chain.

where $H^{(6)}$ represents the six particle exchange term in each hexagon:

$$H^{(6)} = \frac{1}{8} \left(1 + \sum_{\mu < \nu} s_{\mu} s_{\nu} + \sum_{\mu < \nu < \lambda < \rho} s_{\mu} s_{\nu} s_{\lambda} s_{\rho} + s_1 s_2 s_5 s_6 s_9 s_{10} \right) \quad (6)$$

where the first sum goes over all pairs in the hexagon, and the second one goes over all quartets in the hexagon.

3. The recursion relation for the partition function

The partition function of the system is defined in the following way

$$Z = \sum_{\{s_i\}} e^{-H(s_1, s_2, \dots, s_n)/k_B T}, \quad (7)$$

where $H(s_1, s_2, \dots, s_n)$ is the Hamiltonian of the system, k_B is the Boltzmann constant, T is the temperature and the sum goes over all $\{s_1, s_2, \dots, s_n\}$ configurations of the system. Below all the parameters will be rescaled using the Boltzmann constant ($J_2/k_B \equiv J_2$, $J_3/k_B \equiv J_3$, $h/k_B \equiv h$). To obtain recursion relations for the partition function one can separate the kagome ladder into two identical parts (branches) and firstly perform a summation over all spin configurations on each branch, and secondly sum over the central spin variable (see Fig. 1). The summation on each branch yields the same result and such a term only depends on the value of central spin:

$$Z = \sum_{s_0} e^{\frac{h}{T} s_0} g_n^2(s_0) = e^{\frac{h}{T}} g_n^2(+) + e^{-\frac{h}{T}} g_n^2(-), \quad (8)$$

where $g_n(s_0)$ denotes the contribution of each branch. The expression for $g_n(s_0)$ can be written ($s_1 \dots s_{11}$, see Fig. 1) in the form:

$$g_n(s_0) = \sum_{s_1, s_3, \dots, s_{11}} e^{k(s_0, \dots, s_{11})} g_{n-1}(s_{11}), \quad (9)$$

where n is the number of generations and the expression for $k(s_0, \dots, s_{11})$ has the following form:

$$k(s_0, \dots, s_{11}) = -\frac{J_2}{2T} \sum_{18 \text{ pairs}} (1 + s_i s_j) + \frac{J_3}{2T} \sum_{6 \text{ triangles}} (1 + s_i s_j + s_j s_k + s_k s_i) - \frac{J_6}{2T} \cdot H^{(6)} + \frac{h}{T} \sum_{i=1}^{11} s_i. \quad (10)$$

Since g_{n-1} does not depend on s_0, \dots, s_{10} , equation (9) may be obtained as

$$\begin{aligned} g_n(+) &= K(+, +)g_{n-1}(+) + K(+, -)g_{n-1}(-), \\ g_n(-) &= K(-, +)g_{n-1}(+) + K(-, -)g_{n-1}(-), \end{aligned} \quad (11)$$

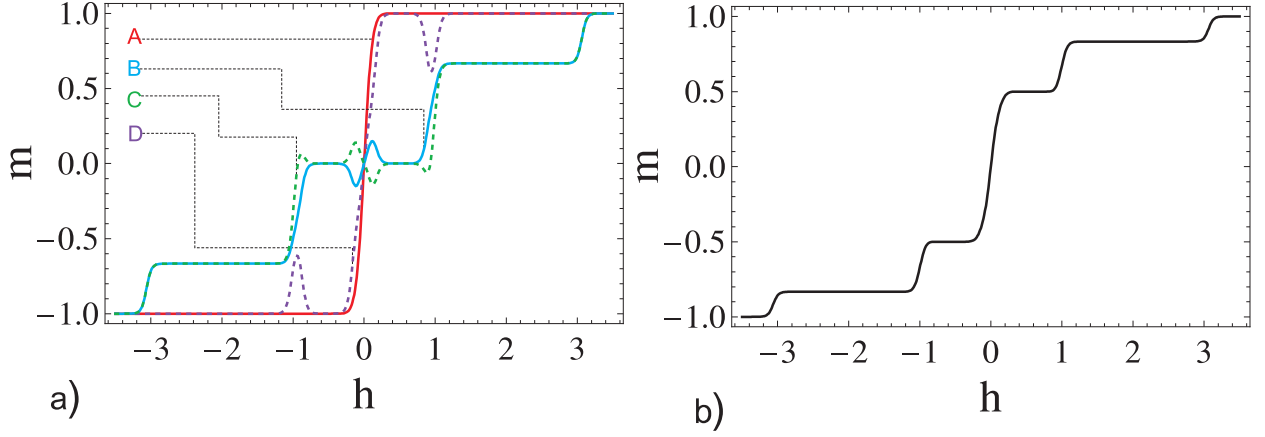


Figure 2:
Magnetization curves for $J_2 = 2mK$, $J_3 = 1.5mK$, $J_6 = 2mK$, $T = 0.04mK$ for a) different sublattices
b) the average magnetization of all sublattices

where we denote $g_n(s_i)$ by $g_n(\pm)$ according to the sign of s_i and $K(s_0, s_{11})$ is the sum of $k(s_0, \dots, s_{11})$ over the ten intermediate spins between s_1 and s_{12}

$$K(s_1, s_{12}) = \sum_{s_2, s_3, \dots, s_{11}} e^{k(s_0, \dots, s_{11})}. \quad (12)$$

The recursion relation is obtained by introducing a new variable $x_n = g_n(+)/g_n(-)$:

$$x_n = \frac{K(+, +)x_{n-1} + K(+, -)}{K(-, +)x_{n-1} + K(-, -)}. \quad (13)$$

4. Magnetization plateaus

The Thermodynamic functions of the system, such as magnetization, can be expressed in terms of x_n . The local magnetization at s_r site is expressed as

$$m = \langle s_r \rangle = \frac{P(s_r)}{Z}, \quad (14)$$

where

$$P(s_r) \equiv \sum_{\{s_i\}} s_r e^{-H(s_1, s_2, \dots, s_n)/k_B T}. \quad (15)$$

By using equation (8) one can write for the central vertex

$$m = \frac{e^{\frac{h}{T}} g_n^2(+) - e^{-\frac{h}{T}} g_n^2(-)}{e^{\frac{h}{T}} g_n^2(+) + e^{-\frac{h}{T}} g_n^2(-)} = \frac{e^{\frac{2h}{T}} x_n^2 - 1}{e^{\frac{2h}{T}} x_n^2 + 1}. \quad (16)$$

To obtain local magnetization for non central vertices one should replace one of two multipliers $g_n(s_1)$ in (8) by formula (9) (see Fig. 1)

$$Z = \sum_{s_0, s_2, \dots, s_{11}} e^{\frac{h}{T} s_0} \cdot e^{k(s_0, \dots, s_{11})} \cdot g_n(s_0) \cdot g_{n-1}(s_{11}). \quad (17)$$

Suppose it is required to find the local magnetization for the r -th site ($r \neq 0, 11$): in that case we must expand sums over s_0 , s_{11} and s_r

$$\begin{aligned} Z = & (K_{+,+}^+ + K_{+,+}^-) \cdot g_n(+)g_{n-1}(+) + (K_{-,+}^+ + K_{-,+}^- + K_{+,-}^+ + K_{+,-}^-) \cdot g_n(+)g_{n-1}(-) + \\ & + (K_{-,-}^+ + K_{-,-}^-) \cdot g_n(-)g_{n-1}(-), \end{aligned} \quad (18)$$

the sum

$$K_{s_0, s_{11}}^{s_r} = \sum_{s_0 \dots s_{r-1}, s_{r+1} \dots s_{11}} e^{\frac{h}{T}s_0} \cdot e^{k(s_0, \dots, s_{11})} \quad (19)$$

is denoted as $K_{\pm, \pm}^{\pm}$ depending on the sign of s_0 , s_{11} and s_r sign. In the same way the expression for $P(s_r)$ may be obtained. The difference is that each $K_{\pm, \pm}^{\pm}$ is replaced by $(-K_{\pm, \pm}^{\pm})$:

$$\begin{aligned} P(s_r) = & (K_{+,+}^+ - K_{+,+}^-) \cdot g_n(+)g_{n-1}(+) + (K_{-,+}^+ - K_{-,+}^- + K_{+,-}^+ - K_{+,-}^-) \cdot g_n(+)g_{n-1}(-) + \\ & + (K_{-,-}^+ - K_{-,-}^-) \cdot g_n(-)g_{n-1}(-). \end{aligned} \quad (20)$$

By using equations (18) and (20) we find the following expression for the magnetization at r -th site in terms of x_n

$$m_r = \frac{(K_{+,+}^+ - K_{+,+}^-) \cdot x_n x_{n-1} + (K_{-,+}^+ - K_{-,+}^- + K_{+,-}^+ - K_{+,-}^-) \cdot x_n + (K_{-,-}^+ - K_{-,-}^-)}{(K_{+,+}^+ + K_{+,+}^-) \cdot x_n x_{n-1} + (K_{-,+}^+ + K_{-,+}^- + K_{+,-}^+ + K_{+,-}^-) \cdot x_n + (K_{-,-}^+ + K_{-,-}^-)}. \quad (21)$$

For fixed values of temperature and exchange parameters the dependence of magnetization on the external magnetic field may be obtained by means of a simple iteration scheme induced by the recursion relations, starting from some initial value x_0 . The thermodynamic limit then corresponds to the asymptotic limit ($n \rightarrow \infty$).

Because of the symmetry of the Hamiltonian, the values of magnetization for some spins are equal: we have in general (See Fig. 1),

$$\begin{aligned} m(s_3) = m(s_4) = m(s_7) = m(s_8) & - A \\ m(s_1) = m(s_2) = m(s_9) = m(s_{10}) & - B \\ m(s_5) = m(s_6) & - C \\ m(s_0) = m(s_{11}) & - D \end{aligned} \quad (22)$$

In Figure 2 magnetization curves are plotted for different sites. As it can be seen from the figure, the magnetization functions have plateaus only for the sublattices B and C.

5. Two dimensional mapping and Lyapunov exponent

It is interesting to calculate the Lyapunov exponent near plateaus but one cannot use recurrent function (13) because it is related to s_1 site. To obtain the recursion relation for the partition function that is related to s_2 site one can separate the kagome chain into two identical parts as shown in Figure 3:

$$Z = \sum_{s_1, s_2, p_1, p_2} N_{p_1, p_2}^{s_1, s_2} \cdot g_n(s_1, s_2) \cdot g_n(p_1, p_2), \quad (23)$$

where

$$N_{p_1, p_2}^{s_1, s_2} = \sum_{s_0} e^{\left\{ \frac{h}{T}(s_1 + s_2 + s_0 + p_1 + p_2) + \frac{J_3 - J_2}{2T} (H^{(2,3)}(s_0, s_1, s_2) + H^{(2,3)}(s_0, p_1, p_2)) - \frac{J_6}{2T} H^{(6)} \right\}} \quad (24)$$

and the contribution of each branch is denoted by $g_n(s_1, s_2)$. The recursion relations for g_n can be obtained by performing eleven ($s_3 \dots s_{13}$, see Fig. 3) summations in the kagome chain:

$$g_n(s_1, s_2) = \sum_{s_{12}, s_{13}} K_{s_{12}, s_{13}}^{s_1, s_2} \cdot g_{n-1}(s_{12}, s_{13}), \quad (25)$$

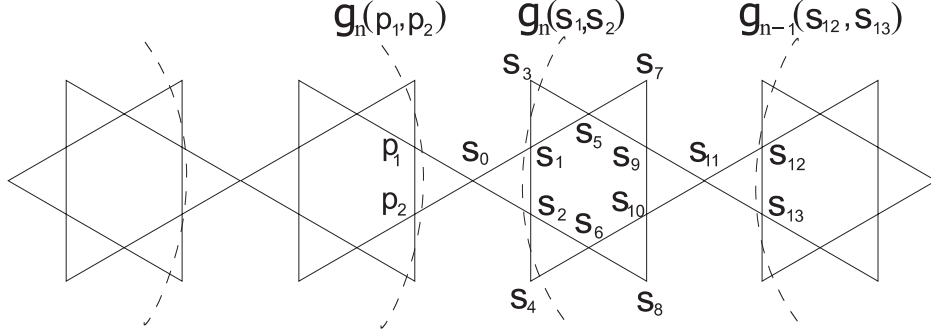


Figure 3: The kagome chain.

where $K_{s_{12}, s_{13}}^{s_1, s_2}$ is as follows

$$K_{s_{12}, s_{13}}^{s_1, s_2} = \sum_{s_3 \cdots s_{11}} e^{\frac{J_3 - J_2}{2T} \sum_{6 \text{ Triangle}} H^{(2,3)} - \frac{J_6}{2T} H^{(6)} + \frac{h}{T} \sum_{i=3}^{13} s_i}. \quad (26)$$

Since $K_{s_{12}, s_{13}}^{s_1, s_2} = K_{s_{12}, s_{13}}^{s_2, s_1}$, $K_{s_{12}, s_{13}}^{s_1, s_2} = K_{s_{13}, s_{12}}^{s_1, s_2}$ one can show that $g_n(+, -) = g_n(-, +)$ and, hance, the recurrence relations are two-dimensional. By introducing $x_n = g_n(+, +)/g_n(-, -)$ and $y_n = g_n(+, -)/g_n(-, -)$ the recursion relations may be written in the following form:

$$\begin{aligned} x_n = \Phi(x_{n-1}, y_{n-1}), \quad \Phi(x, y) &= \frac{K_{+,+}^{+,+}x + 2K_{+,+}^{+,-}y + K_{-,+}^{+,-}}{K_{+,+}^{-,-}x + 2K_{+,+}^{-,-}y + K_{-,+}^{-,-}}, \\ y_n = \Psi(x_{n-1}, y_{n-1}), \quad \Psi(x, y) &= \frac{K_{+,+}^{+,-}x + 2K_{+,+}^{+,-}y + K_{-,+}^{+,-}}{K_{+,+}^{-,-}x + 2K_{+,+}^{-,-}y + K_{-,+}^{-,-}}. \end{aligned} \quad (27)$$

The magnetization can be expressed in terms of x_n, y_n with due regard for (23) and (24)

$$m(s_1) = \frac{\sum_{s_1, s_2, p_1, p_2} s_1 \cdot N_{p_1, p_2}^{s_1, s_2} \cdot g_n(s_1, s_2) \cdot g_n(p_1, p_2)}{\sum_{s_1, s_2, p_1, p_2} N_{p_1, p_2}^{s_1, s_2} \cdot g_n(s_1, s_2) \cdot g_n(p_1, p_2)}. \quad (28)$$

Taking into account that $N_{p_1, p_2}^{s_1, s_2} = N_{p_1, p_2}^{s_2, s_1} = N_{p_2, p_1}^{s_1, s_2} = N_{s_1, s_2}^{p_1, p_2}$, we get after the expansion of sums:

$$m(s_1) = \frac{N_{+,+}^{+,+}x_n^2 + 2N_{+,+}^{+,-}x_ny_n - 2N_{-,+}^{+,-}y_n - N_{-,+}^{-,-}}{N_{+,+}^{+,+}x_n^2 + 4N_{+,+}^{+,-}x_ny_n + 4N_{+,+}^{+,-}y_n^2 + 2N_{-,+}^{+,+}x_n + 4N_{-,+}^{+,-}y_n + N_{-,+}^{-,-}}. \quad (29)$$

Magnetization curves calculated by formulae (29) and (21) with $r = 1$ coincide. Relations (27) permit the calculation of Lyapunov exponents near the plateaus: in the two-dimensional space they have the form

$$\lambda_{1,2} = \lim_{N \rightarrow \infty} \frac{1}{N} \ln (\text{eigenvalues}\{\mathbf{\Lambda}(x_1, y_1) \cdot \mathbf{\Lambda}(x_2, y_2) \cdots \mathbf{\Lambda}(x_N, y_N)\}), \quad (30)$$

where $\mathbf{\Lambda}(x_i, y_i)$ is Jacobian matrix evaluated at the (x_i, y_i) point

$$\mathbf{\Lambda}(x_i, y_i) = \begin{pmatrix} \frac{\partial \Phi}{\partial x} & \frac{\partial \Phi}{\partial y} \\ \frac{\partial \Psi}{\partial x} & \frac{\partial \Psi}{\partial y} \end{pmatrix} \bigg|_{x_i, y_i}. \quad (31)$$

The only subtle point in the estimation of Lyapunov exponents [45, 46, 47] is in the rescaling procedure in each iteration to avoid the numerical overflow. The results of calculation are shown in Fig. 4 with the corresponding magnetization function: it is seen in the figures that the maximum Lyapunov exponent also exhibits plateaus. Moreover, for the maximum Lyapunov exponent the location of magnetization plateaus coincide with those of magnetization curves.

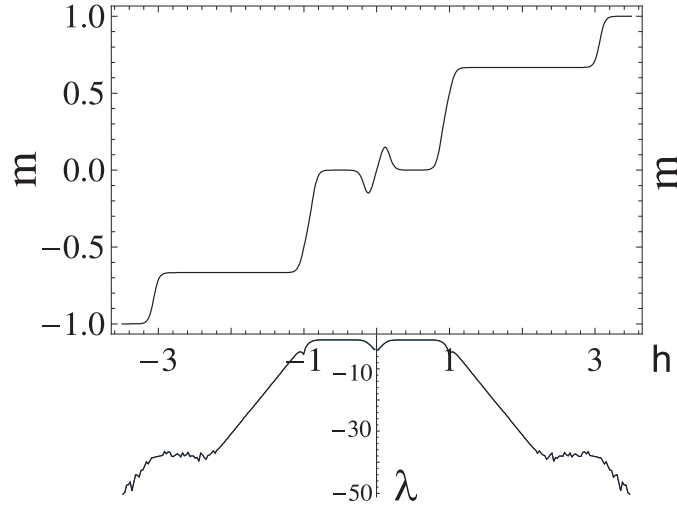


Figure 4: Coincidence of magnetization plateaus and the maximum of Lyapunov exponent.

Conclusions

In the present paper the theory of dynamical systems has been used to study magnetization on the kagome chain. In a strong external magnetic field the Ising model has been considered instead of the Heisenberg one for the case of two, three and six-site exchange interactions. Exact recursion relations have been derived for the partition function. The magnetization curves for different temperatures and exchange parameters were obtained and the kagome chain was observed to split into four sublattices with different magnetizations. Two of them exhibit plateaus at zero and $2/3$ of the saturation field value at low temperatures and certain exchange parameters. A multidimensional mapping was deduced to study the maximum Lyapunov exponent near the plateaus and it was shown that the location of plateaus on the maximal Lyapunov exponent and for magnetization was the same.

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